Trelliscope: A System for Detailed Visualization in the Deep Analysis of Large Complex Data

Ryan Hafen*
Pacific Northwest National Lab
Karin Rodland
Pacific Northwest National Lab

Luke Gosink
Pacific Northwest National Lab
Kerstin Kleese-Van Dam
Pacific Northwest National Lab

Jason McDermott
Pacific Northwest National Lab
William S. Cleveland
Purdue University

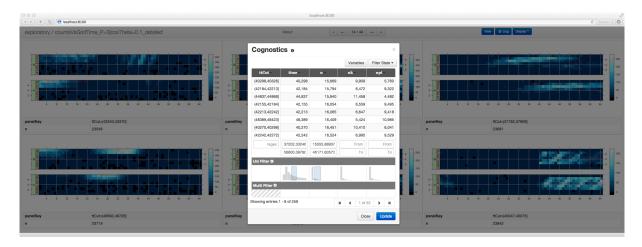


Figure 1: Screenshot of the Trelliscope viewer showing a display created during analysis of high intensity physics data. In the configuration shown, 6 panels are displayed per screen, which are sorted and filtered according the parameters specified in the cognostics pane.

ABSTRACT

Trelliscope emanates from the Trellis Display framework for visualization and the Divide and Recombine (D&R) approach to analyzing large complex data. In Trellis, the data are broken up into subsets, a visualization method is applied to each subset, and the display result is an array of panels, one per subset. This is a powerful framework for visualization of data, both small and large. In D&R, the data are broken up into subsets, and any analytic method from statistics and machine learning is applied to each subset independently. Then the outputs are recombined. This provides not only a powerful framework for analysis, but also feasible and practical computations using distributed computational facilities. It enables deep analysis of the data: study of both data summaries as well as the detailed data at their finest granularity. This is critical to full understanding of the data. It also enables the analyst to program using an interactive high-level language for data analysis such as R, which allows the analyst to focus more on the data and less on code. In this paper we introduce Trelliscope, a system that scales Trellis to large complex data. It provides a way to create displays with a very large number of panels and an interactive viewer that allows the analyst to sort, filter, and sample the panels in a meaningful way. We discuss the underlying principles, design, and scalable architecture of Trelliscope, and illustrate its use on three analysis projects in proteomics, high intensity physics, and power systems engineering.

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*e-mail: ryan.hafen@pnnl.gov

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1 Introduction

The Trellis visualization framework [2] provides an effective approach to detailed visualization of complex data. It has been widely used for data analysis as a way to meaningfully visualize both summary and detailed data. Currently, the most used implementation is the R package, Lattice [17].

In Trellis Display, the data are divided into subsets based on conditioning variables, and a plotting method is applied to each subset. The resulting plot for each subset is displayed on a "panel". Current Trellis implementations render the panels on a single display that takes the form of a three-dimensional array with rows, columns, and "pages". The whole process is controlled by a number of display methods that can be simply specified by the user. Implementations have provided a programming capability using the graphics language of the system that allows a user to specify almost any visualization method as the panel method. All of this enables a user to uncover the structure of data even when the structure is quite complicated. Trellis Display is discussed in Section 2.

Like all other analytic methods for data analysis, Trellis Display becomes difficult to use effectively for large complex data. There are two problems: (1) how to efficiently generate and organize a large number of panels; and (2) how to view and interact with many panels.

Trelliscope is an extension of Trellis that solves these problems. The extensions are described in Section 3. Problem (1) is solved by employing the Divide and Recombine (D&R) approach to large complex data, which is discussed in Section 3.1. Problem (2) is solved by making methods of sampling subsets a part of Trelliscope. We describe sampling and the use of "cognostics" in Section

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14. ABSTRACT

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3.2. Then, Section 4 introduces the design and implementation of Trelliscope. Section 5 illustrates its usage in three applications.

2 TRELLIS DISPLAY

Divide and Recombine (D&R), Trellis Display, and Trelliscope all have as a fundamental aspect a division of data into subsets, and then a recombination. We begin with an illustration of division and Trellis Display with a very small dataset.

Figure 2 is a Trellis Display of data from a 1930s experiment at the Minnesota Agricultural Experiment Station. At 6 sites, 10 varieties of barley were grown in each of 2 years. The data collected for the experiment are the yields for all combinations of the three factors — site, variety, and year — so there are 120 observations. In the figure, there are two conditioning variables: site and year. Site has 6 values and year has 2, so there are 12 combinations of site and year. The data are divided into 12 subsets by the 12 combinations. The visualization analytic method applied to each subset is a dotplot. Each panel of the display is this dotplot for one subset.

This Trellis display allows us to study the the dependence of yield on variety conditional on site and year, and how the relationship changes with the values of the conditioning variables. This turns out to be an exceptionally powerful mechanism for analysis of data, both small and large. Often, a number of Trellis displays are made with different conditioning variables; for example, we can plot yield and site given variety and year.

The barley data demonstrate the power of D&R. They were published by R. A. Fisher in his book, *Statistical Methods for Research Workers*, and through the decades became a canonical dataset used to illustrate many new numerical statistical methods. Despite the many re-analyses through time, it was not until the use of Trellis Display in their analysis 60 years later that a major error in the reported data was discovered [6]. This display gives a first clue, an anomaly at Morris.

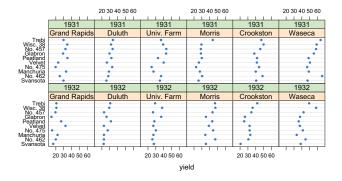


Figure 2: A Trellis display of the barley data.

There are many visualization methods that are employed to enhance the effectiveness of Trellis Display. While these choices are largely up to the user to specify, a good Trellis implementation will provide mechanisms to specify and explore these choices with ease. More details on these and other considerations can be found in [11] and [2].

3 EXTENDING TRELLIS

Trelliscope extends Trellis Display to large complex data, enabling the efficient generation of displays with a very large number of panels that can be easily and effectively viewed. To achieve this we use the Divide and Recombine (D&R) approach to large complex data to generate the displays, and sampling of subsets to make the number of panels manageable.

3.1 Divide and Recombine

3.1.1 Introduction

Divide and Recombine (D&R) is a statistical approach to the analysis of large complex data [10]. The data are divided into subsets. Analytic methods are applied to each of the subsets, and the outputs of each method are recombined to form a result for the entire data. This provides computational feasibility and practicality.

There are two categories of analytic methods: statistical methods (including machine learning methods), whose output is numeric and categorical, and visualization methods, whose output is visual. For a visualization method, the recombination is a visual display that assembles the panels for viewing across subsets. For a statistical analytic method, the recombination results in numeric and categorical values. For example, suppose we carry out logistic linear regression on subsets. The outputs are the estimates of the regression coefficients, and statistical information about the estimates. The recombination can be unweighted means of the subset coefficient estimates, or means weighted by estimates of their variances.

The D&R division and recombination methods used for an analytic method are critical to the success of the D&R result. We seek "best" division and recombination methods that suit the analysis task at hand. In many cases, we are interested in studying the behavior of individual subsets of the data partitioned by categorical variables. An example is the visualization of the barley data, where each subset is determined by the year and site. Divisions can also be chosen such that each subset is a random partition of the data, where each subset can be thought of as an experiment. With such divisions, in many cases we can obtain analytic recombination results that serve as approximations that are very close or exactly the same as what we could have gotten had we been able to apply the analytic method to all of the data directly.

3.1.2 Two Goals

One goal for D&R is deep analysis of large complex data: detailed, comprehensive analysis that does not lose important information in the data. Deep analysis requires visualization of the data at their finest granularity, not just visualization of summaries. This was established in the 1960s by the pioneers of data visualization for model building such as John Tukey, Frank Anscombe, Cuthbert Daniel, and George Box. We can do this with small data. For large complex data, should we wave the white flag, surrendering to the size and complexity, and visualize just summaries? Would that not be a step backward? Large complex data should not get a pass.

A second goal is the analyst being able to use a well-designed interactive language for data analysis. This can reduce substantially the time an analyst spends programming with the data compared with using a lower-level language. There is a very clear metric: the fraction of the time the analyst spends thinking about programming versus the fraction of time spent thinking about the data. We seek to minimize the former. The language also needs to be powerful, allowing a tailoring of the analysis to the data. The language needs to provide access to the 1000s of statistical and analytic methods that exist today. R [15], does a very good job in efficiency for the analyst, programming power, and accessing methods.

3.1.3 The Computational Environment

What makes D&R work is that the computations for the application of an analytic method to the subsets can be run in parallel with no communication among them. D&R can exploit parallel distributed computational environments like Hadoop with its MapReduce compute engine and Hadoop distributed file system. D&R makes it feasible for a data analyst to apply almost any statistical or visualization method to large complex data.

Of course, the data analyst does not want to program in Hadoop's native language, Java. RHIPE, the R and Hadoop Integrated Programming Environment, enables the analyst to write Hadoop

MapReduce jobs completely in R [9]. RHIPE has two parts. A core, written in R and Java, that communicates with Hadoop. The second part is a prototype domain-specific language for D&R in R, available as a package named datadr [13]. This software provides a simple interface for specifying division and recombination methods. The datadr methods provide a layer on top of RHIPE, allowing the analyst to only think in terms of meaningful division and recombination methods, hiding the details of MapReduce from the user. Also, datadr has been designed with the goal in mind of linking to other computing and storage backends.

Trelliscope has been implemented in the the D&R computational environment of R and datadr. There are a number of potential backends. Thus far we have used RHIPE/Hadoop, which provides for scaling to large complex data, efficiently creating Trelliscope displays with many panels.

3.2 Sampling Panels with Cognostics

A natural approach to viewing many panels is simply scrolling through all pages of panels tiled across a screen. This alone can be very powerful, but can become unrealistic when the number of panels is large. In our own applications, the number of subsets range from thousands to millions.

Our approach to viewing a large number of panels in a meaningful way is to compute metrics on the data being plotted in each panel that identify interesting qualitative or quantitative attributes, and then sample, filter, or sort the panels based on these metrics. Here, we loosely refer to any such metric as a "cognostic", a Tukey term for "computer guiding diagnostics" [5].

What constitutes an "interesting attribute" of a subset? In most cases, this is left up to the analyst to determine for the visualization at hand. A cognostic metric is simply the result of any computation the analyst can think of that exploits some behavior in the data being visualized. Examples are simple statistical metrics such as the mean, standard deviation, quantiles, range, and number of observations. If a model fit is being plotted, a goodness-of-fit metric for the model fit for the subset can be a meaningful cognostic. Other examples are the percentage of values exceeding some limit, number of times a specific value is seen, difference between means of two groups of data, etc.

There is no specific set of steps for specifying these types of cognostics. Finding meaningful cognostics is typically an iterative process. The analyst creates a panel plotting function, applies it to a few subsets, studies the resulting plots, and determines a candidate set of cognostics that might provide a meaningful space for navigating the collection of all panels. Then the analyst applies the panel and cognostics function to all subsets and views the results.

Cognostics can also come from work in the interesting related area of research on scatterplot diagnostics, or "scagnostics" [21]. Scagnostics are cognostics specifically for scatterplots in which algorithms provide metrics for specific types of interesting behavior, such as "outlying", "skewed", "clumpy", "striated", etc. [21]. These cognostic metrics have more of a flavor of the computer trying to tell the analyst what is interesting in a scatterplot (probably more true to what Tukey had in mind), as opposed to the analyst-defined cognostics described previously.

Cognostics are specified and attached to a Trelliscope display within the programming environment, as they require specification of potentially complex algorithms to return the desired metrics. The analyst provides a function that takes a subset of data as input and returns a list of cognostic attributes. An example of how a display is created along with the cognostics is shown in Section 4.

There are different ways cognostics can be used to interact with the panels of a Trelliscope display. For very exploratory views of the display, a panel viewer can present the set of cognostics to the analyst and allow them to sort and filter the panels based on the different cognostic attributes. This results in a "focused sampling" of panels based on different metrics of interest. Our implementation of such a Trelliscope viewer is described in Section 4.

In cases where we would like to conduct a more controlled study of the panels of a large display, we can take representative samples of panels based on distributions of cognostics. A representative sample covers the joint region of values of a set of cognostic variables. In most cases the variables are known to have an effect, and we seek to study their effect within the region of the multidimensional space that they collectively occupy. For example, suppose 10^6 subsets have variable sample sizes n. Suppose from each subset we get an estimate of a parameter, and 5000 bootstrap values of the estimate to describe the sampling distribution of the estimator for the subset. Suppose we want to study the normality of the bootstrap distribution for each subset by a normal quantile plot, and how it changes with n. Of course our expectation is that the estimator gets closer to normal as n increases. We could check normality by making normal quantile plots for 1000 subsets whose values of n on the log scale are as close to equal as possible. Such representative sampling could be specified either in a Trelliscope viewer or from the analysis programming environment.

4 DESIGN AND IMPLEMENTATION OF TRELLISCOPE

The Trellis extension concepts introduced in the previous section are quite straightforward – the idea is to use a distributed computing interface to create the panels and leverage cognostics and sampling to interactively view the panels. However, inserting these ideas into an implementation that provides meaningful interactivity and an efficient workflow for a data analyst, while being interoperable with a distributed storage and computing backend, is not trivial.

We have created an R implementation of the Trellis extensions, called Trelliscope. As a system, Trelliscope builds upon D&R by providing methods to apply panel and cognostic functions to divided datasets to create displays with many panels, providing a web-based viewer that allows users to interact with the panels, all with minimal effort. For example, users can sort and filter millions of panels using a wide variety of cognostics values. The filtered panels are tiled on a screen where the user can then rapidly page through them.

To support this at-scale flexibility for visualization, Trelliscope takes as input a dataset divided into subsets using the divide () method from the datadr D&R package [13]. This data can either be a divided local data frame or a divided dataset on the Hadoop distributed file system (HDFS). A prepanel function can be applied to the data to determine axis limits for each panel. If limits are not specified, scales are chosen such that the data fills the panel. The analyst then specifies a plot function and a cognostics function to be applied to each subset and sends these to a command makeDisplay(). This function applies the panel and cognostics functions to each subset and stores the results. Trelliscope employs R as a visualization system to create the plots and compute the cognostics. By using the R-based interfaces of base R graphics, lattice, or ggplot [20, 17], it is possible to create nearly any visual representation that a user requires. There are several options for how plots and cognostics are stored, which are discussed in greater detail later in Sections 4.1.1 and 4.1.2.

4.1 Hardware Architecture

Trelliscope can work on a single workstation operating on inmemory data frames in R. When dealing with very large data sets, Trelliscope can interface with scalable, distributed hardware architectures. For example, Figure 3 shows how Trelliscope can operate seamlessly with very large datasets stored on HDFS. Our analysis environment has been set up in a way similar to that of Figure 3, except that the web server and cognostics server are both running on the master node of the Hadoop cluster.

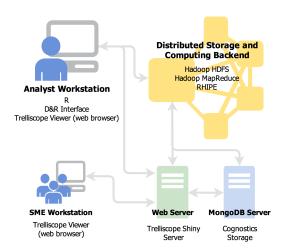


Figure 3: Distributed architecture of Trelliscope. Trelliscope is capable of running on a single workstation, but has the ability to run in a distributed architecture, one possibility of which is shown here. All analysis work is done on the analyst's workstation in R, and the D&R interface and Trelliscope R package coordinate communication with the other services. Other users, such as subject-matter experts (SMEs) can access the viewer through a web browser.

4.1.1 Panel Rendering

We have investigated and implemented several options for panel rendering and storage. There are two major classes of panel rendering possibilities: 1) prerender and store raster images on disk, HDFS, or MongoDB; 2) render panel images on-the-fly. In the latter case, pointers to each subset on disk are stored in the image's place and the images are rendered on-the-fly by reading the associated data when requested by the viewer.

The advantage of rendering on-the-fly is much quicker initial creation of a display (only cognostics are computed), as well as the ability to dynamically modify the panel function from within the viewer. This particularly makes sense when there are millions of subsets and the probability of viewing all subsets is very low, in which case there is not much sense in precomputing all of them. It typically is not expensive in terms of compute time or storage space to compute cognostics for every subset, even when the number of subsets is in the millions. The only possible downside to the render-on-the-fly approach is the case when the plot function is very expensive to apply. In that case, it can be worth the time expense to pre-generate the plots so that time isn't spent on rendering during the viewing process.

In our implementation, the viewer knows how to link to a panel image or data through a special cognostic automatically computed for each display called panelKey. Panel images or data can be uniquely located through the combination of the display name and panel key. Panel data or images stored on HDFS are stored as key/value pair Hadoop mapfiles [19] with the key being the panel key. The images or data can then be rapidly retrieved by key when the viewer requests them. For panel images stored on disk, the files are named according to panel key and are retrievable by name.

4.1.2 Cognostics Storage

Cognostics for a display can be stored either as an R data frame on disk or as a collection in a database. The R data frame storage approach is the simplest and does not require additional hardware or software to be available aside from R on a workstation. The potential drawback to this approach is that it does not scale well beyond a few million subsets as the viewer must load the entire cognostics data frame into memory to show the display.

Storing the cognostics in a database is another option that provides several benefits over a data frame approach. Most databases

will provide the ability to index columns of the database for fast filtering, while not being required to be loaded into memory on the web server. We have chosen MongoDB as a database option for storing cognostics in our system. MongoDB scales very easily and has a flexible aggregation framework that we plan to leverage to perform different viewer-directed transformations and aggregations of cognostics.

4.2 Creating a Display in R

Creating a display from an R instance is as simple as calling the makeDisplay() function and specifying 1) a divided input dataset, 2) a name for the display, and 3) a plot function for the panels. Other optional settings (e.g., display group, axis limits, and a cognostics function) can be specified as well. With respect to data types, makeDisplay() can handle different classes of divided data objects (e.g. local data frame or HDFS) and there are different parameter defaults for how plots and cognostics are stored based on the input type. Detailed documentation about all of the options with examples is provided in the online documentation [14].

An example of creating a display could look like this:

```
makeDisplay(
  data = gridCounts,
  group = "exploratory",
  name = "gridCounts",
  desc = "Number of grid hits over time",
  lims = list(x="free", y="free"),
  plotFn = gcPlot,
  cogFn = gcCog,
  plotDim = list(height = 200, width = 800),
  storage = "hdfsData")
```

Here, gridCounts is a divided HDFS data object. We have created and tested a plot function gcPlot and a cognostics function gcCog that we are specifying to be applied to the each subset of this data. We specify the x and y axis limits to be "free". The storage option is "hdfsData", meaning that only cognostics will be computed, including a panelKey that will be used to fetch data and render on-the-fly in the viewer.

Prior to calling makeDisplay(), there are functions that aid the analyst in specifying the panel axis limits. A prepanel() function computes the axis limits for each subset and returns them. The analyst can visualize the limits with a special R plot method to get a feel for the distribution of the axis limit values. This can be helpful in discovering subsets with large outlying values which are sure to abound when the data is very large, and the analyst can specify to trim outliers so that they do not inflate the axis limits of all panels.

4.3 The Trelliscope Viewer

The Trelliscope viewer is a web application written in R using the R Shiny [16] package. The server for the viewer can either run on the user's workstation or on a web server. The viewer is accessed through a web browser. Shiny provides communication from the web browser to a live R session on the web server through a WebSocket connection, providing an interactive user interface controlled by JavaScript.

4.3.1 Panel View

The panel view is the main component of the viewer; Figure 4 shows the panel view for a display created during the analysis of high intensity physics data where the user has specified to view six panels per screen. Once the user has selected a display to view, the panel view tiles the panels of the chosen display across the screen. Left and right keys or the navigation buttons on the header bar provide simple navigation through the collection of panels.

By clicking the "view" button, the analyst can specify how many panels are to be viewed in a single screen and can also specify

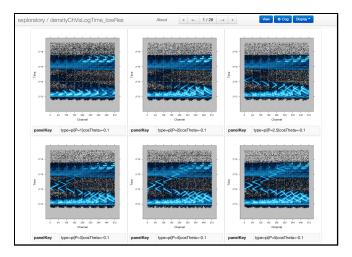


Figure 4: Screenshot of the panel view of the Trelliscope viewer for a display created during the analysis of high intensity physics data.

whether cognostic values should be displayed alongside each panel. There is also the "view" option to edit the panel plotting function for displays that are not pre-rendered. This ability to dynamically change what is being plotted is an additional benefit to not pre-rendering the plots. The user can react to what is being seen in the panels directly through the viewer (e.g. adding a reference line) without going back to R to recreate the entire display. An example screenshot of the view pane is shown in Figure 5.



Figure 5: Screenshot of view pane of the Trelliscope viewer. The panel plot editing tab is visible.

4.3.2 Cognostics Interaction

A major feature of the Trelliscope viewer is the ability to sort and filter panels according to the cognostics. Clicking the "Cog" button brings up an interactive table that displays the cognostics variables. Clicking column headers in the cognostics panel allows for sorting, with multi-column sorting available with shift-click. In addition to sorting, there are filters available for each variable. Regular expressions can be used to filter qualitative variables and numerical ranges can be used to filter quantitative variables. A screenshot of the cognostics pane for a display is shown in Figure 6. This figure depicts an example of filtering and sorting where operations done in the cognostics pane determine how the panels will be displayed back in the panel view.

The cognostics pane also allows for interactive visual filtering of cognostics for quantitative variables. Visual filtering is useful in

Cognostics	0			
			Variables	Filter State ▼
panelKey –	time	n∨	nk-	npi –
ttCut=(34122,34145]	34,122	60,724	34,094	26,63
ttCut=(34145,34169]	34,145	58,718	32,577	26,14
ttCut=(34169,34193]	34,169	57,270	31,803	25,46
ttCut=(34193,34217]	34,193	55,844	30,740	25,10
ttCut=(35497,35522]	35,497	55,446	28,198	27,24
ttCut=(35448,35472]	35,448	55,219	27,841	27,37
ttCut=(35522,35546]	35,522	55,218	28,532	26,68
ttCut=(35472,35497]	35,472	55,051	28,091	26,96
regex	34112.31818	From	From	From
	74877.69696	То	То	То
Uni Filter 3				
Multi Filter 6				
Showing entries 1 - 8 of	of 1134	H	∢ 1 of 14	2 > N
			Clos	e Update

Figure 6: Screenshot of the cognostics pane in the Trelliscope viewer. In addition to panelKey, 4 cognostics variables are visible. The time cognostic has been range filtered and the filtered cognostics are sorted in reverse order by the cognostic variable n.

that it can help the user identify regions of interest in the cognostics space using the distribution of the cognostic as a visual cue. The visual filters are created using d3.js [3].

For univariate filtering, the user can click the histograms at the bottom of the cognostics table (see Figure 6). This activates the histogram so that users can select a range of the histogram's values; a screenshot of this type of selection is shown in Figure 7.

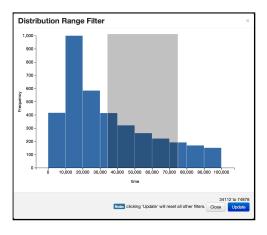


Figure 7: Screenshot of the interactive univariate histogram cognostic filter in the Trelliscope viewer.

Multivariate filtering is also possible. In the cognostics pane's "Multi Filter" section, the user can select two variables and bring up an interactive scatterplot from which a bivariate range of values can be identified to filter on. If there are more than 5,000 cognostics, a hexagonal binning [4] is computed and plotted instead of individual points. In the future, the viewer will support more than two variables by using projection pursuit to project the multivariate data onto a two-dimensional plane which the user can then interact with. An example of bivariate filtering is shown in Figure 8.

4.3.3 Viewing related displays

It is very common to create multiple displays for the same division of the data. When this is the case, it is useful to view multiple

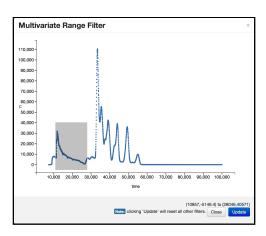


Figure 8: Screenshot of the interactive bivariate cognostic filter in the Trelliscope viewer.

displays side-by-side for each subset. Trelliscope provides a way to do this by keeping track of which displays were created from the same division. By selecting the "Displays" button and selecting "Related Displays" from the menu, the user can select any number of related displays to be shown in the viewer.

5 APPLICATIONS

We have employed the principles behind Trelliscope in many projects [12, 22]. Here, we discuss three recent projects that have made direct use of the Trelliscope implementation. The main goal of this paper is to introduce the Trelliscope methodology and implementation, and therefore we are not able to go into details for these applications. Our aim is to briefly illustrate the use of Trelliscope in real-world data analysis projects and demonstrate a few use cases where it was an integral part of deep analysis.

5.1 Power Systems Data Cleaning and Event Detection

Sensors called Phasor Measurement Units (PMUs) provide power grid operators with the status of the electric power grid at various geographical locations at a very high frequency, 30-60 times per second. Our analysis covered a data set of 1.5 years of data from 38 PMUs, a data set 2TB in size. The data consists of about 1.5 billion time points with measurements from 38 PMU locations, where each PMU records on average 14 measurements. These measurements include the measured frequency at which the grid is operating as well as several phase angle measurements.

The initial goal for our analysis was to build event detection algorithms for specific grid activities of interest such as generator trips and grid islanding. Our initial inquiry for the data was simply to understand the behavior of each series over time. As all behaviors of interest are time-local, we chose a subsetting scheme of time intervals that are short enough to be able to process and visualize at high enough time resolution, but long enough to ensure that we capture the time-local behavior within subsets. Based on these requirements, we settled on 5 minute time intervals for subsetting. There are about 158,000 subsets of the data, and when additionally splitting out by location, there are about 6 million subsets.

We investigated the data using Trelliscope to create and view time series plots of the subsets. Trelliscope provided a way for us to have immediately at our fingertips a detailed view of any time sequence of the 2TB dataset. Figure 9 shows two panels of one of the time series displays created. The frequency of the grid across a 5-minute segment of time is shown, with a series for each of the 38 PMUs overplotted. The frequency reported for each PMU generally follows the same trend over time.

We iteratively developed a collection of useful cognostics for this display. Simple attributes that provide for temporal sorting and filtering include the start time of the time interval and derived attributes such as time of day, day of week, etc. Other simple attributes include the number of missing values and number of times the frequency exceeds a limit specified by power systems engineers to be alarming or physically impossible. The time series vary around a trend that changes over time. To capture that variability, we specified a cognostic that removes the trend by fitting a local polynomial regression to the time series and computes a robust measure of the standard deviation of residual values of this fit. This cognostic helps point us to subsets of the data where the variability around the trend is unusually large or small. Another useful cognostic we computed was the steepest slope of the fitted trend across the 5-minute interval, which helped us investigate time periods of extreme changes in frequency.

Sorting and filtering on cognostic variables would typically bring subsets to our attention where other interesting behavior was occurring not captured by, but correlated with, the cognostics. Some of these behaviors were so rare that it is doubtful that they would have been discovered without the ability to interactively look at the data at the greatest level of detail. A large proportion of the behaviors we uncovered were deemed to be erroneous records. The combination of Trelliscope for detailed views with the analytical recombination methods of D&R enabled us to identify, validate, and build algorithms to remove these records from the data to focus on the event detection. Many of the types of erroneous records had gone unnoticed in several prior analyses where tools like D&R and Trelliscope were not available.

Another notable use-case of Trelliscope was in fine-tuning our generator trip algorithm. Based on examples of known trips, we were able to identify characteristics of a generator trip: all frequency measurements experience a sharp sudden drop followed by a gradual recovery. We constructed features from the data that captured these types of behaviors, but were not certain at which point the combination of feature metrics constituted a bona fide generator trip. We used the metrics to procure a candidate set of over 3000 time periods in which we thought a generator trip might have occurred. This data constituted a new division with each subset containing the data corresponding to the suspected generator trip. We created a Trelliscope time series display of the data and presented them to a domain expert to view and classify using the Trelliscope viewer. Classification narrowed the list down to about 500 verified trips and from this narrowed list we were able to create a rulesbased algorithm for detecting generator trips. A screenshot of the Trelliscope viewer being used for this purpose is shown in Figure 9.

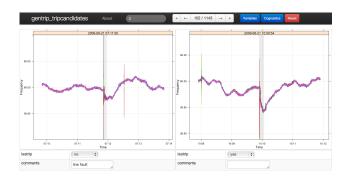


Figure 9: Trelliscope viewer being used to view and verify generator trips in a power systems engineering application.

5.2 High Intensity Physics Particle Classification

In a high intensity physics application, we are looking at detecting and differentiating between two sub-atomic particles, pion and

kaon, that are present during a single 100ns event from simulated data that models a detector in the Belle II experiment [8]. Within a single event, the numbers of these particles, their ratio to each other, and the energy distribution of each particle type is key to identifying inconsistencies in the Standard Model of particle physics.

This is an ongoing project, but our initial task, in anticipation of real data becoming available in the coming years, is to see if it is feasible to do kaon / pion classification from simulated data. We are able to stochastically simulate data from a variety of possible scenarios. From a high-level, the scenario of interest begins when a kaon or pion particle hits the exterior of the detector and releases a small array of photons into one of the detector's quartz chamber The particles themselves enter the detector at a known momentum, P, and propagate photons radially at an unknown angle, θ . The particles bounce around the detector until they hit a sensor grid defined by 64×8 channels (labeled 1, ..., 512). We have simulated hundreds of thousands of events from 168 combinations of P, θ , and particle type (kaon/pion). The simulation reports the hit time and location on the sensor. The complete realizations we are currently studying generate about 12GB of data but we will soon be looking at much larger collections of events. This is not nearly as much data as in our previous example, but still enough that we cannot tackle this data with traditional approaches.

In our first step, we divide the data into subsets for each combination of P, θ , and particle type in order to study the distribution of hit times and locations on the sensor grid according to channel. This results in a manageable 168 subsets. One Trelliscope display we created on this division is a hexagonal binned scatterplot of time vs. channel. An example of this for pions with $cos(\theta) = 0.1$ and P ranging from 1 to 5 (left to right, top to bottom) is seen in Figure 4. Initially, cognostics for this display were simply specified to be the values of P, θ , and particle type that define the subset. We viewed the display in the Trelliscope viewer, choosing 2 panels per page and sorting the panels first based on P, then θ , then particle type. This allowed us to view the kaon and pion scatterplots side-by-side for fixed P and θ , and then page through all 168 panels making visual comparisons as we progress through different levels of θ and then P. Viewing in this way, we noticed that for small P, it is easy to visually distinguish kaons and pions, but as P increases (from $P \ge 3$), the two begin to look very similar.

To further investigate the kaon / pion behavior, we partitioned the data by time. More specifically, we choose one set of parameters, P = 3 and $cos(\theta) = 0.1$ to study and contrast kaon / pion behavior in detail. An initial look at this case over time led us to desire a finer time resolution and hence more sample runs. We generated 1 million sample runs for this case and divided the data up into 3739 subsets according to equal-width log time intervals. One display we created for this data is a heat map of the hit distribution within each time chunk for each of kaon and pion, plotted according to the actual grid layout of the sensor. An example of this display can be seen in the background of Figure 1. For this display, we computed cognostics for the start time of the interval, the number of kaon hits, the number of pion hits, and the difference between kaon and pion hits. Our first view of this display was simply quickly paging through the panels in time order. This view helped us notice that there are time periods in which a clear signal is present on the sensor, which moves around on the sensor over time. The activity comes in bursts, and the signal is only present when the activity is high, verified by looking at the scatterplot of the cognostics of number of hits vs. time (see Figure 8). Viewing this display also gave us a better view of the differences between kaon and pion and we were able to see many times where the signal was visibly very different between the two. Based on our observations, we constructed a simple Bayes classifier for any new sample. The sample hits are matched to the time partitions of our time-divided data, and then based on the distribution of the training data in that time period, we compute the probability that the point is a kaon or pion given its hit location on the grid. We found that if we weight these classifications based on the time regions where the difference between kaon and pion is most pronounced, we can get accurate classification in the 90% range. While here we have omitted several of the iterations and steps in this process, Trelliscope and the datadr package played a crucial role in doing this analysis effectively in a very short time.

5.3 Proteomics Biomarker Discovery

The goal of a proteomics research problem we have been involved with is to extract meaningful signatures of biological processes from peptide and protein abundance data. The process of biomarker discovery and characterization provides opportunities both for purely statistical and expert knowledge-based approaches. In this project we investigated the use of Trelliscope in an effort to improve integration of the two.

We used proteomics data from a mouse model of chronic obstructive pulmonary disease (COPD) that involves deletion of a gene, ADA. Animals with ADA+/- are controls (no disease) ADA+/+ are diseased. We analyzed data from plasma samples of control and disease groups over time to study biomarkers for COPD. The abundance data underwent an extensive preprocessing procedure, resulting in data for 2,927 peptides which were rolled up into 414 proteins. Statistical and functional clustering tools were applied to the data, forming potential groups of biomarkers.

We created a visual representation of the data in Trelliscope to present to a domain expert. We divided the protein data into subsets by protein and likewise for the peptide data. The panel function for each protein or peptide displays the abundance over time by disease and control groups. An example of two panels from the protein display is shown in Figure 10. The dots represent the abundances for each subject, while the crosshairs and lines denote the mean abundance at each time point for each group and its progression over time. The top and bottom sets of boxes colored in gray and green indicate whether a statistically significant difference exists between the two groups at each time point, the top row for a G-test (test for presence/absence) and the bottom for a t-test for difference between group means [18]. A statistically significant positive difference between control and disease for the given test at the given time point, gray means insignificant, and red means a statistically significant negative difference. These boxes helped create a visual cue that can be rapidly digested while paging through many panels.

We computed several cognostics for each panel. Some simple statistical cognostics derived from the data in each subset include the following: number of total, ADA-/-, and ADA+/- observations in the panel, average difference between ADA+/- and ADA-/- before and after day 34, t-test and g-test p-values on each day, slope of ADA-/- and ADA+/- abundance over time. We merged external domain-specific data with our subsets to obtain cognostics providing more information about the protein, including protein annotation and function, cluster assignment from hierarchical clustering, enriched functional cluster assignment and gene functional classification from DAVID [7], and assigned generalized biological process from GO [1].

Using these cognsotics, data analysts and domain experts were able to interact with the panels in many ways. Panels were sorted and filtered on proteins of interest, protein functions of interest, etc. to help the domain expert understand what the data had to say. Panels were also sorted by statistical significance trends of interest, such as abundances that are not significantly different in the beginning and become significant over time. Another interaction was filtering the panels based on the clustering results and determining if the resulting protein groupings made any sense, as well as trying to determine if there was anything apparent in the data that would explain and provide some interpretability of the protein groupings

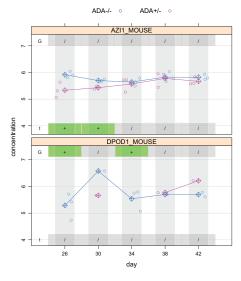


Figure 10: Two panels from a display of protein abundance vs. time for disease (ADA+/-) and control (ADA-/-) groups.

selected.

This analysis facilitated by Trelliscope provided valuable insight into the data for the domain experts in several key aspects. Visualization of the peptides (portions of the whole protein) contributing to quantitation of key proteins was evaluated. In several cases it was apparent that there were two trends in the peptides mapping to one protein indicating that the mapping was incorrect. Grouping of the proteins into functional groups was used to identify subgroups for incorporation into a classification algorithm that allowed identification of improved biosignatures of disease in the COPD samples.

The data for this example is by far the smallest (less than 10MB) and illustrates the utility of Trelliscope when the data is not large. Detailed views of the data still required panels for thousands of subsets and thus benefitted from the interactivity of Trelliscope.

6 DISCUSSION AND FUTURE WORK

Trelliscope provides a framework for scalable detailed, interactive visualization of large complex data. It has been developed out of necessity from analysis of many real-world large complex datasets and has proven to be immensely useful.

Trelliscope is a research effort that to this point has been mainly focused on the architecture and practicality of a scalable Trellis Display system. In the future, we would like to give much more attention to the design and features of the viewer.

The main focus of future work on the viewer will be sampling and cognostics. We envision an interface that allows the analyst to specify different sampling schemes of the panels. We also anticipate new cognostic types that provide new ways to interact with the data. One of these is relational cognostics, where the cognostic for one panel is a reference to another panel or panels either in the same display or in other displays. Such cognostics could be displayed and interacted with in the viewer through a network graph.

We also envision more options with how the quantitative and qualitative cognostics are interacted with. This would include more complex visual interactions with multiple cognostic variables.

We have given consideration to the idea of using more modern web-based technologies to create and render the panel images. This could bring a new level of interactivity. However, we feel there is sufficient power (and ease of use) for the analyst by allowing them to stick to tools they are familiar with to create the panel-level plots while still being able to have rich interactions with these plots at the cognostics level.

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REFERENCES

- M. Ashburner, C. A. Ball, J. A. Blake, D. Botstein, H. Butler, J. M. Cherry, A. P. Davis, K. Dolinski, S. S. Dwight, J. T. Eppig, et al. Gene ontology: tool for the unification of biology. *Nature genetics*, 25(1):25–29, 2000.
- [2] R. A. Becker, W. S. Cleveland, and M.-J. Shyu. The visual design and control of trellis display. *Journal of Computational and Graphical Statistics*, 5(2):123–155, 1996.
- [3] M. Bostock, V. Ogievetsky, and J. Heer. D³ data-driven documents. Visualization and Computer Graphics, IEEE Transactions on, 17(12):2301–2309, 2011.
- [4] D. B. Carr, R. J. Littlefield, W. Nicholson, and J. Littlefield. Scatterplot matrix techniques for large n. *Journal of the American Statistical Association*, 82(398):424–436, 1987.
- [5] W. Cleveland. The Collected Works of John W. Tukey: Graphics 1965-1985, volume 5. Chapman & Hall/CRC, 1988.
- [6] W. S. Cleveland. Visualizing Data. Hobart Press, Chicago, 1993.
- [7] G. Dennis Jr, B. T. Sherman, D. A. Hosack, J. Yang, W. Gao, H. C. Lane, R. A. Lempicki, et al. David: database for annotation, visualization, and integrated discovery. *Genome Biol*, 4(5):P3, 2003.
- [8] T. et al. Belle II Technical Design Report, 2010.
- [9] S. Guha. Computing Environment for the Statistical Analysis of Large and Complex Data. PhD thesis, Purdue University Department of Statistics, 2010.
- [10] S. Guha, R. Hafen, J. Rounds, J. Xia, J. Li, B. Xi, and W. S. Cleveland. Large complex data: divide and recombine (d&r) with rhipe. *Stat*, 1(1):53–67, 2012.
- [11] S. Guha, R. P. Hafen, P. Kidwell, and W. S.Cleveland. Visualization Databases for the Analysis of Large Complex Datasets. *Journal of Machine Learning Research*, 5:193–200, 2009.
- [12] S. Guha, P. Kidwell, A. Barthur, W. S. Cleveland, J. Gerth, and C. Bullard. A Streaming Statistical Algorithm for Detection of SSH Keystroke Packets in TCP Connections. In R. K. Wood and R. F. Dell, editors, Operations Research, Computing, and Homeland Defense. Institute for Operations Research and Management Sciences, 2011.
- [13] R. Hafen. "datadr" github documentation. http://hafen.github.io/datadr/. Accessed: 2013-05-11.
- [14] R. Hafen. "trelliscope" github documentation. http://hafen.github.io/trelliscope/. Accessed: 2013-05-11.
- [15] R Core Team. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria, 2012. ISBN 3-900051-07-0.
- [16] RStudio and Inc. shiny: Web Application Framework for R, 2013. R package version 0.5.0.
- [17] D. Sarkar. Lattice: multivariate data visualization with R. Springer Verlag, 2008.
- [18] B.-J. M. Webb-Robertson, L. A. McCue, K. M. Waters, M. M. Matzke, J. M. Jacobs, T. O. Metz, S. M. Varnum, and J. G. Pounds. Combined statistical analyses of peptide intensities and peptide occurrences improves identification of significant peptides from ms-based proteomics data. *Journal of proteome research*, 9(11):5748–5756, 2010.
- [19] T. White. Hadoop: The definitive guide. O'Reilly Media, Inc., 2012.
- [20] H. Wickham. ggplot2: elegant graphics for data analysis. Springer Publishing Company, Incorporated, 2009.
- [21] L. Wilkinson, A. Anand, and R. Grossman. High-dimensional visual analytics: Interactive exploration guided by pairwise views of point distributions. Visualization and Computer Graphics, IEEE Transactions on, 12(6):1363–1372, 2006.
- [22] B. Xi, H. Chen, W. S. Cleveland, and T. Telkamp. Statistical Analysis and Modeling of Internet VoIP Traffic for Network Engineering. *Electronic Journal of Statistics*, 4:58–116, 2010.